Triethylenetetramine
112-24-3 | DTXSID9023702

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.94e-11 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 4.96e-01

Confidence level: 9.13e-01

Nearest Neighbors from the Training Set

Image not found
Hexadecane
Measured: 2.49e-11
Predicted: 2.20e-11

Image not found
Pentadecane
Measured: 2.22e-11
Predicted: 2.07e-11

Image not found
Tetradecane
Measured: 1.92e-11
Predicted: 1.90e-11

Image not found
Tridecane
Measured: 1.60e-11
Predicted: 1.64e-11

Image not found
Dodecane
Measured: 1.42e-11
Predicted: 1.31e-11